polarizable force fields id greatly facilitated by extensive use of quantum mechanical data for both fitting and testing purposes.

3099-Pos Board B146

Single Molecule Reaction Kinetics within Femtoliter Volume Containers

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We create and observe controlled single molecule chemical reactions within femtoliter containers called hydrosomes. Hydrosomes are stable aqueous nanodroplets suspended in a low index-of-refraction fluorocarbon medium. The index of refraction mismatch between the nanodroplets and fluorocarbon is such that individual hydrosomes can be optically trapped. Using optical tweezers, the hydrosomes are held within a confocal observation volume, and we interrogate the encapsulated molecule by means of fluorescence excitation. Hydrosome encapsulation has an important advantage over liposome encapsulation techniques in that hydrosomes fuse on contact, thereby mixing the encapsulated components. Optical tweezers are used to manipulate the hydrosomes and to induce a fusion event. Custom fabricated microfluidic channels are used to sort the hydrosomes containing different molecule species. We demonstrate the use of hydrosomes as microreactors by fusing two hydrosomes, each containing a complementary single strand of DNA, and observing the subsequent hybridization via FRET (Fluorescence Resonance Energy Transfer).

3100-Pos Board B147

Photoexcitation Spectrum of Protonated Tyrosine in Vacuum and Theoretical Interpretation

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Photodepletion spectrum of gaseous protonated tyrosine molecules was obtained at 150 K by UV laser spectroscopic technique in conjunction with mass spectrometry and interpreted by theoretical methods. The spectrum exhibits distinct three bands separated each other by about 800 . Four stable conformers of the molecular ion were determined by the quantum mechanical density functional theory and their electronic transition energies were obtained by a semi-empirical quantum chemistry calculation. The whole pattern of the spectrum was reproduced very well by a combination of theoretical methods, the second order cumulant expansion, ZINDO/S calculation, molecular dynamics simulation, and a semi-classical time-correlation function approach. The three spectral bands turned out to arise from the vibronic transition of two vibrational modes constituted by the ''benzene breathing'' mode and a torsional mode of the amino acid backbone. It is suggested that the major factor of the spectral broadening is not conformational disorder but the thermal fluctuation of the most stable conformer. Excellent agreement between the experimental and theoretical spectra exemplifies the validity of the theoretical methods applied for the present molecular system.

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Prediction of Hofmeister ion effects on biopolymer processes

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At moderate to high concentrations, salt ions exert a wide range of effects on protein folding and other protein processes, from extremely destabilizing (GuH^+, SCN^-) to very stabilizing (SO_4^{2-}). The Hofmeister series is a qualitative ranking of these effects, originally based on the effectiveness of salts as protein precipitants and subsequently observed for other processes including creating air-water surface and dissolving hydrocarbons in water. Recently surface spectroscopy, molecular dynamics simulations and molecular thermodynamic analysis of surface tension and model compound solubility data have all provided evidence that local accumulation or exclusion of individual salt ions, relative to bulk concentrations, is responsible for their Hofmeister effects. In particular, application of a novel two-domain salt ion partitioning model (SPM) to analyze effects of Hofmeister salts on the surface tension of water and on hydrocarbon and peptide solubility (Pegram & Record, J. Phys. Chem. B 112, 9428 (2008); 111, 5411 (2007)) provides a quantitative molecular thermodynamic description of the individual partitioning of salt cations and anions at uncharged interfaces, with predictive capability. This analysis shows that the Hofmeister rank order of ions arises from their interactions with nonpolar surface. Surface-bulk partition coefficients of ions obtained from hydrocarbon and amide model compound solubility data, together with a coarse-grained description of functional groups that make up molecular surfaces, allow the quantitative prediction of Hofmeister (noncoulombic) salt effects on micelle formation, protein folding, protein crystallization and DNA helix formation.

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3102-Pos Board B149

Hofmeister Effects on Beetle Antifreeze Protein Activity Enhancement

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Antifreeze proteins (AFPs) noncolligatively depress the nonequilibrium freezing point of a solution. A difference between the melting and freezing points is termed as thermal hysteresis (TH). Some low-molecular-mass solutes can affect the TH values of AFPs. The TH enhancement effects of series low-molecular-mass enhancers on an AFP from the beetle *Dendroides canadensis* (DAFP) have been extensively investigated. However, the mechanisms of the enhancement effects of the enhancers are still not well understood. The adsorption-inhibition mechanism is a generally accepted mechanism of AFPs. In this work, the effect of a series of neutral salts on salting out DAFP on ice is treated by a simple classical theory. In the presence of these anions, DAFPs are salted out on ice, which may lead a larger surface DAFP coverage than that in the absence of these anions. Therefore, the TH value of DAFP will enhance in the presence of a series of simple anions. The TH values of DAFP in the presence of the series of anions assessed by Differential Scanning Calorimetry (DSC) are in an excellent agreement with the theoretical results from the classical theory. Our results show that the Hofmeister effect may be one of the potential mechanisms for AFP enhancers. Besides Hofmeister ion interactions, the anion enhancers may also interact with DAFP/water/ice through other ways. Further discussions are given.

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Solvation in Solvent-Cosolvent Mixtures

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The volumetric properties of solutes, including their partial molar volume, compressibility, and expansibility, are known to be determined by and, therefore, sensitive to the entire spectrum of solute-solvent interactions. However, applications of volumetric measurements to study of solvation of solutes in binary solvents consisting of the principal solvent and a cosolvent are almost nonexistent. This deficiency reflects the lack of an adequate theoretical framework to rationalize the measured volumetric observables in terms of solute-principal solvent and solute-cosolvent interactions. To address this deficiency, we present in this work a simple statistical thermodynamic model describing solute thermodynamics in binary solvents. Based on the model, we derive relationships that link the partial molar volumetric properties of solutes with the extent and intensity of interactions of a solute with the principal solvent and the cosolvent. If the approximation of uniform solvation is introduced, the derived formalism can be simplified to a form that can be readily employed for practical treatment of experimental volumetric data on small solutes and/or individual, chemically homogeneous atomic groups. As an example, we use this simplified formalism to rationalize the volumetric properties of the zwitterionic amino acid glycine in concentrated urea solutions. In general, the theoretical development presented in this work opens the way for systematic applications of volumetric measurements to quantitative characterization of solute-solvent interactions in complex solvents.

3104-Pos Board B151

Effect of Ionic and Non-ionic Co-Solutes on the Activity of β-Galactosidase

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The hydrolysis of the lactose analog o-Nitrophenyl-beta-D-Galactopyranoside into o-Nitrophenol and beta-D-Galactose by the action of beta-Galatosidase is a well known enzymatic reaction. We have studied this reaction with varying concentrations of substrate in the presence of several ionic and non-ionic cosolutes considered chaotropes and kosmotropes, and examined their effects on the enzyme activity. In the presence of increasing concentrations of up to 1 M NaCl, beta-Galactosidase showed an activity that was barely affected by the salt concentration and was basically similar to that under stripped conditions. In contrast, in the presence of NaI, while at concentrations of 0.1 M NaI and below the effect on the enzyme activity was comparable to that of 0.1 M NaCl, in the presence of 1 M NaI the enzyme showed a marked deactivation. This fact suggested that the difference in effects was caused by the presence of iodide ions. On the other hand, the activity of this enzyme was also investigated in the presence of several polyols differing in the number of hydroxyl groups. The kosmotropes used were glycerol (3), erythritol (4), xylitol